

HIGH RESOLUTION INFRARED DATASETS
USEFUL FOR VALIDATING STRATOSPHERIC MODELS

Curtis P. Rinsland
Atmospheric Sciences Division
NASA Langley Research Center
Hampton, Virginia

514-46
12029

First Annual High-Speed Research Workshop
Williamsburg, Virginia
May 14-16, 1991

PRECEDING PAGE BLANK NOT FILMED

INTRODUCTION

An important objective of the High Speed Research Program (HSRP) is to support research in the atmospheric sciences that will improve our basic understanding of the circulation and chemistry of the stratosphere and lead to an interim assessment of the impact of a projected fleet of HSCTs (High Speed Civil Transports) on the stratosphere. As part of this work, critical comparisons between models and existing high-quality measurements are planned. These comparisons will be used to test the reliability of current atmospheric chemistry models. In this paper, two suitable sets of high-resolution infrared measurements are discussed.

ATMOS/SPACELAB 3 DATASET

The ATMOS (Atmospheric Trace Molecule Spectroscopy) experiment was designed to obtain 0.015-cm^{-1} resolution infrared solar occultation spectra of the atmosphere from which the vertical distributions of a large number of minor and trace molecular constituents of the upper atmosphere could be retrieved. The experiment was flown for the first time in the spring of 1985 as part of the Shuttle Spacelab-3 mission. Nineteen complete atmospheric occultations were recorded, twelve sunsets between latitudes of 25°N and 32°N , and seven sunrises between 45°S and 48°S latitude, on April 29 to May 1, 1985. For an overview of the ATMOS experiment and the results of the Spacelab 3 mission see the paper by Farmer (ref. 1).

The profiles for several dozen atmospheric constituents and pressure and temperature have been retrieved from the ATMOS middle atmosphere data. Because the spectra were recorded with broadband filters, chemically linked molecular species were often measured simultaneously, thus providing a unique opportunity to study the partitioning within key chemical families. The ATMOS/Spacelab 3 results are reviewed below. References which give the retrieved profiles and their uncertainties are cited.

Chlorine and Fluorine Budgets. Stratospheric profiles of 11 chlorine- and fluorine-containing source, sink, and reservoir molecules were derived from the Spacelab 3 measurements. The molecules are CCl_2F_2 (chlorofluorocarbon 12), CCl_3F (chlorofluorocarbon 11), CHClF_2 (chlorofluorocarbon 22), CCl_4 , ClONO_2 , HCl , HF , CF_4 (chlorofluorocarbon 14), COF_2 , CH_3Cl , and SF_6 . Results for the source gases have been reported by Zander et al. (ref. 2). Measurements of the sink gases were reported by Raper et al. (ref. 3). Recently, the profiles of HCl , HF , and ClONO_2 have been revised based on improvements in the spectroscopic database and the processing of the ATMOS spectra (ref. 4). The identification and results for SF_6 are reported in ref. 5.

Odd Nitrogen Budget. Profiles of the following odd nitrogen molecular species were derived from the Spacelab 3 measurements: NO , NO_2 , HNO_3 , HO_2NO_2 , N_2O_5 , and ClONO_2 . The analysis included normalized factors that correct for the rapid diurnal variations of NO and NO_2 at sunrise and sunset. These factors were computed with a photochemical

model. The profiles of N_2O_5 were measured for the first time at both sunrise (48°S) and sunset (28°N). The profiles are reported in ref. 6, except for the updated measurements of N_2O_5 which are in ref. 7.

Key Minor Gases. The ATMOS profiles of CH_4 , N_2O , CO , H_2O , and O_3 cover a wide region of the middle atmosphere (ref. 8). For example, the H_2O profiles extend from 14 to 86 km and the O_3 profiles cover 14 to 94 km. The ATMOS sunset profiles of CH_4 and N_2O show a fold in their vertical distributions which is probably the result of dynamics. The sunrise profiles do not show the fold. Recently, stratospheric profiles of the isotopic species H_2^{18}O , H_2^{17}O , HDO , and CH_3D have also been retrieved (ref. 9).

Other Gases. Profiles of the nonmethane hydrocarbons C_2H_6 and C_2H_2 (ref. 10) and the molecules HCN and OCS (ref. 11) have also been reported from the ATMOS/Spacelab 3 observations.

GROUND-BASED MEASUREMENTS OF TOTAL COLUMNS

High-resolution ($\sim 0.01 \text{ cm}^{-1}$) solar absorption spectra recorded with the McMath Fourier transform spectrometer on Kitt Peak (altitude 2.09 km, 31.9°N, 111.6°W) have been analyzed to deduce total column amounts of HF on 93 different days and HCl on 35 different days between May 1977 and June 1990 (ref. 12). The results indicate a rapid increase in total HF and a more gradual increase in total HCl with both trends superimposed on a seasonal cycle with an early spring maximum and an early fall minimum. The peak-to-peak amplitudes of the seasonal cycle are equal to 25% for HF and 13% for HCl.

These results are of interest since current estimates indicate that the supersonic fleet may be operating in the early 21st century when the atmospheric concentrations of several key gases will be different than they are today. Sensitivity studies to assess the effects of these aircraft will necessarily require generating scenarios for future emissions including the projected emissions of supersonic and subsonic aircraft. The Kitt Peak measurements provide an opportunity to compare model calculations with a time series of accurate measurements for which there are fairly reliable data on emission histories and photo-oxidation rates for the source molecules. The model-predicted and measured total columns, increase rates, and seasonal cycles can be compared.

Of the two species, HF is better suited for the model-measurement comparisons because there probably are no significant tropospheric HF sources. In contrast, in the boundary layer, HCl is produced primarily by the interaction of SO_4 and NO_3 ions with NaCl in ocean spray, and to a lesser extent by surface anthropogenic emissions, such as the burning of plastics and emissions from certain industrial processes. Because of these sources, it is necessary to specify a nonzero surface level HCl flux in model calculations to simulate total column observations. Previous model-model comparisons showed large scatter in the calculated HCl total columns because of differences in the adopted surface level HCl concentration (ref. 13). Therefore, to

make meaningful comparisons with the Kitt Peak data, the tropospheric contribution will need to be prescribed in the model runs based on the observations, which indicate that the tropospheric contribution is about 15% of the total column.

Additional long-term IR spectroscopic observations of HF and HCl have been obtained from the Jungfraujoch station in the Switzerland (altitude 3.58 km, 46.5°N, 8.0°E). At the present time, R. Zander of the University of Liège and collaborators are reanalyzing the early data and extending the baseline of total column measurements based on recently collected solar spectra. It is unclear whether or not this updated database will be available in time for the upcoming HSRP model-measurement comparisons.

REFERENCES

1. Farmer, C. B.: High Resolution Infrared Spectroscopy of the Sun and Earth's Atmosphere from Space. *Mikrochim. Acta* [Wien], vol. III, 1987, pp. 189-214.
2. Zander, R.; Rinsland, C. P.; Farmer, C. B.; and Norton, R. H.: Infrared Spectroscopic Measurements of Halogenated Source Gases in the Stratosphere with the ATMOS Instrument. *J. Geophys. Res.*, vol. 92, 1987, pp. 9836-9850.
3. Raper, O. F.; Farmer, C. B.; Zander, R.; and Park, J. H.: Infrared Spectroscopic Measurements of Halogenated Sink and Reservoir Gases in the Stratosphere with the ATMOS Instrument. *J. Geophys. Res.*, vol. 92, 1987, pp. 9851-9858.
4. Zander, R.; Gunson, M. R.; Foster, J. C.; Rinsland, C. P.; and Namkung, J.: Stratospheric ClONO_2 , HCl , and HF Concentration Profiles Derived from Atmospheric Trace Molecule Spectroscopy Experiment Spacelab 3 Observations: An Update. *J. Geophys. Res.*, vol. 95, 1990, pp. 20,519-20,525.
5. Rinsland, C. P.; Brown, L. R.; and Farmer, C. B.: Infrared Spectroscopic Detection of Sulfur Hexafluoride (SF_6) in the Lower Stratosphere and Upper Troposphere. *J. Geophys. Res.*, vol. 95, 1990, pp. 5577-5585.
6. Russell, J. M. III; Farmer, C. B.; Rinsland, C. P.; Zander, R.; Froidevaux, L.; Toon, G. C.; Gao, B.; Shaw, J.; and Gunson, M.: Measurements of Odd Nitrogen Compounds in the Stratosphere by the ATMOS Experiment on Spacelab 3. *J. Geophys. Res.*, vol. 93, 1988, pp. 1718-1736.
7. Rinsland, C. P.; Toon, G. C.; Farmer, C. B.; Norton, R. H.; and Namkung, J. S.: Stratospheric N_2O_5 Profiles at Sunrise and Sunset from Further Analysis of the ATMOS/Spacelab 3 Solar Spectra. *J. Geophys. Res.*, vol. 94, 1989, pp. 18,341-18,349.
8. Gunson, M. R.; Farmer, C. B.; Norton, R. H.; Zander, R.; Rinsland, C. P.; Shaw, J. H.; and Gao, B.-C.: Measurements of CH_4 , N_2O , CO , H_2O , and O_3 in the Middle Atmosphere by the Atmospheric Trace Molecule Spectroscopy Experiment on Spacelab 3. *J. Geophys. Res.*, vol. 95, 1990, pp. 13,867-13,882.
9. Rinsland, C. P.; Gunson, M. R.; Foster, J. C.; Toth, R. A.; Farmer, C. B.; and Zander, R.: Stratospheric Profiles of Heavy Water Vapor Isotopes and CH_3D from Analysis of the ATMOS Spacelab 3 Infrared Solar Spectra. *J. Geophys. Res.*, vol. 96, 1991, pp. 1057-1068.

REFERENCES (continued)

10. Rinsland, C. P.; Zander, R.; Farmer, C. B.; Norton, R. H.; and Russell, J. M.: Concentrations of Ethane (C_2H_6) in the Lower Stratosphere and Upper Troposphere and Acetylene (C_2H_2) in the Upper Troposphere Deduced from Atmospheric Trace Molecule Spectroscopy/Spacelab 3 Spectra. J. Geophys. Res., vol. 92, 1987, pp. 11,951-11964.
11. Zander, R.; Rinsland, C. P.; Farmer, C. B.; Namkung, J.; Norton, R. H.; and Russell, J. M. III: Concentrations of Carbonyl Sulfide and Hydrogen Cyanide in the Free Upper Troposphere and Lower Stratosphere Deduced from ATMOS/Spacelab 3 Infrared Solar Occultation Spectra. J. Geophys. Res., vol. 93, 1988, pp. 1669-1678.
12. Rinsland, C. P.; Levine, J. S.; Goldman, A.; Sze, N. D.; Ko, M. K. W.; and Johnson, D. W.: Infrared Measurements of HF and HCl Total Column Abundances above Kitt Peak, 1977-1990: Seasonal Cycles, Long-Term Increases, and Comparisons with Model Calculations, J. Geophys. Res., in press, 1991.
13. Two-Dimensional Intercomparison of Stratospheric Models, NASA Conference Publication 3042, section 3.4.2, 1989, pp. 64.

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.

1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE April 1992	3. REPORT TYPE AND DATES COVERED Conference Publication	
4. TITLE AND SUBTITLE First Annual High-Speed Research Workshop			5. FUNDING NUMBERS WU 537-01-22-01	
6. AUTHOR(S) Allen H. Whitehead, Jr., Compiler				
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) NASA Langley Research Center Hampton, VA 23665-5225			8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) National Aeronautics and Space Administration Washington, DC 20546-0001			10. SPONSORING/MONITORING AGENCY REPORT NUMBER NASA CP-10087, Part 1	
11. SUPPLEMENTARY NOTES				
12a. DISTRIBUTION/AVAILABILITY STATEMENT LIMITED DISTRIBUTION until April 30, 1994 Subject Category 02			12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words) This publication is in four volumes and represents the compilation of papers presented at the First Annual High-Speed Research Workshop held in Williamsburg, Virginia, on May 14-16, 1991. This NASA-sponsored workshop provided a national forum for presenting and discussing important technology issues related to the definition of an economically viable, and environmentally compatible High-Speed Civil Transport. The Workshop and this publication are organized into 13 sessions, with Session 1 presenting NASA and Industry overviews of the High-Speed Civil Transport Program. The remaining sessions are developed around the technical components of NASA's Phase I High-Speed Research Program, which addresses the environmental issues of atmospheric emissions, community noise and sonic boom. Because of the criticality of the materials and structures technology area, and the long-term nature of the supporting research requirements, a session was added in this area to capture the ongoing work at NASA Lewis and NASA Langley and within industry.				
14. SUBJECT TERMS atmospheric science, high lift, laminar flow control, sonic boom, aeroacoustics, supersonic transport, ozone, community noise			15. NUMBER OF PAGES 513	
			16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT Unclassified	18. SECURITY CLASSIFICATION OF THIS PAGE Unclassified	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT	

NSN 7540-01-280-5500

Standard Form 298 (Rev. 2-89)
Prescribed by ANSI Std. Z39-18,
298-102

